**Req #28325**

**Job Description**

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| **Posting Title:** | Scientist I, Chem & Mol Therapeutics |
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| **Job Description:** | Computational Chemist with expertise in Free Energy simulations of receptor-ligand complexes and other approaches of ligand binding energy calculations as well as structure-based and ligand-based drug design methodologies to generate models and provide expert analysis of SAR data to support decision making for lead identification and optimization with excellent communication skills, strong leadership skills, and ability to work independently and in close collaboration with medicinal chemists,.  The preferred candidate would have demonstrated expertise in several of the following skills:  • Molecular Dynamics and Free Energy simulations of receptor-ligand complexes  • Structure-based approaches for iterative improvement of compound potency and selectivity  • Virtual screening, fragment-based approaches, data mining of internal and external databases to Identify new starting points for small molecule projects  • Virtual library design and enumeration  • Analysis of high throughput screening results and large data sets  • Visualization of SAR data to help medicinal chemists  • Ligand-based design methodologies (pharmacophore modeling/QSAR)  • Proficiency in programming/scripting and HPC/Cloud computing  • Knowledge of neurodegenerative and neuroinflammatory drug targets |
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| **Qualifications:** | Proven expertise in Free Energy Simulations and protein-ligand binding energy calculations as well as structure-based / ligand-based drug design methods and their application as demonstrated by publications and conference presentations. Expertise in two or more of the following software packages: Schrödinger, OpenEye, CCG and Vortex. A solid background in Statistics, Chemistry and/or Biology is a plus. |
| **Education:** | Ph.D. in Computational Chemistry, or any branch of Chemistry and related disciplines with 0 - 5 years of post-doctoral experience in academia or pharmaceutical industry are required. |
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